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Title: Molybdenum Benchmark Update

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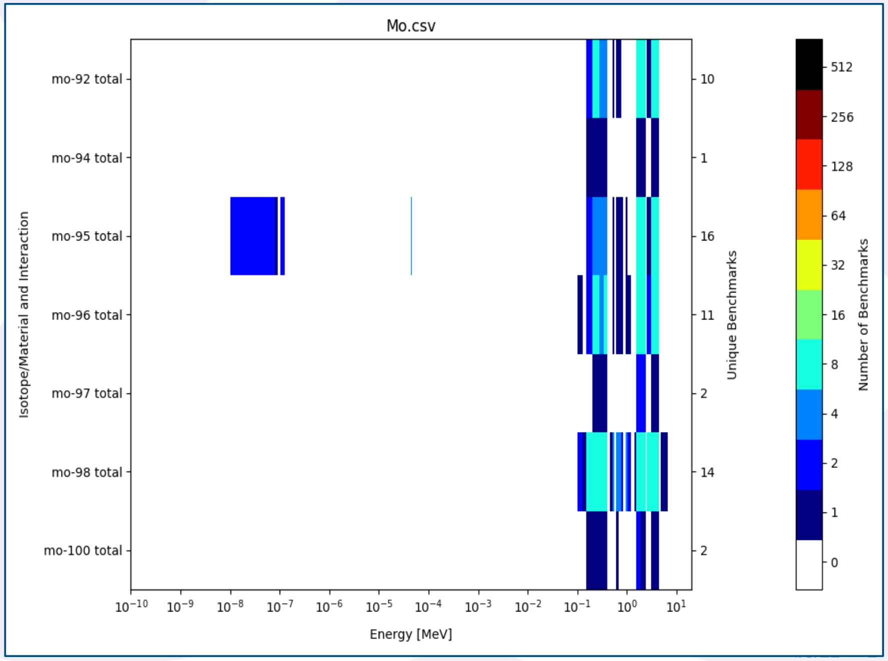
Molybdenum Benchmark Update

Cole Kostelac, Nicholas Thompson, Rene Sanchez, Jesson Hutchinson

July 20, 2021

Review of Motivations

- Molybdenum (Mo) isotopes found in HALEU fuels, space reactor applications, fission product inventories
- ^{95}Mo is one of the 15 main absorbing fission products in light water reactors
- New differential measurements of isotopic Mo cross sections in unresolved resonance region (URR) from RPI need validation*
- New and future Mo cross sections from IRSN and JAEA at J-PARC need validation**
- There are few benchmarks sensitive to Mo
- Only one intermediate benchmark



*R. Bahran et al, "Isotopic molybdenum total neutron cross section in the unresolved resonance region", Phys Rev C, **92**, 024601 (2015) https://journals.aps.org/prc/pdf/10.1103/PhysRevC.92.024601

I. Duhamel et al, "Measurement, evaluation and validation of molybdenum cross sections", EPJ Web of Conferences **247, 09007 (2021) https://doi.org/10.1051/epjconf/202124709007

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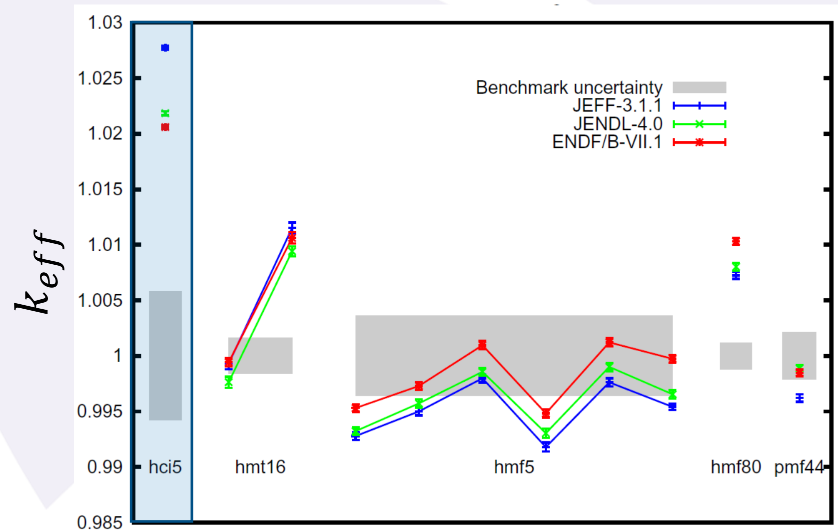
Existing Molybdenum Benchmarks

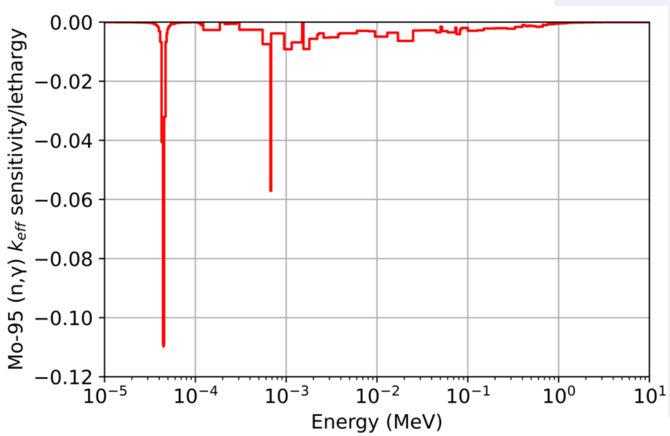
- Only one intermediate molybdenum sensitive benchmark in the ISCBEP handbook, HEU-COMP-INTER-005
- Conducted in Russian Federation in the 1980’s, accepted to handbook in 2002
- Large bias between computational and experimental results



ICSBEP benchmarks containing Mo

Category	N	ENDF/B-VII.1	JENDL-4.0	JEFF-3.1.1
heu-comp-inter	1	2060	2185	2774
heu-met-therm	2	503	353	541
heu-met-fast	7	-5	-227	-316
pu-met-fast	1	-152	-113	-378

Average values for C/E - 1 (in pcm) for benchmarks containing Mo using MCNP6.1. N is the number of benchmarks in the category.

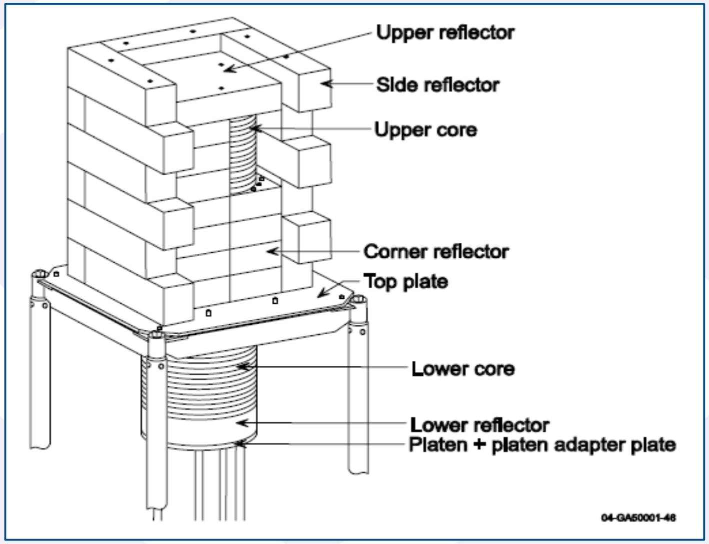


HEU-COMP-INTER-005 ^{95}Mo(n,γ) sensitivity

HEU/Molybdenum Experimental Design

- COMET vertical lift assembly
- Core will consist of stacking Jemima plates (HEU metal), molybdenum plates, and moderator plates.
- Varying the thicknesses of the molybdenum and moderating plates will be used to shape the energy spectrum of the system
- Unit geometries repeated until criticality is reached

COMET with radial and axial copper reflector



HMF-072

Unmoderated unit geometry

Moderated unit geometry

Goals

Fast (x1)

Intermediate (x3)

Thermal (x1)

Case 1
- “Fast Case”
- Unmoderated, copper reflected
- Maximize ^{95}Mo(n,γ) sensitivity in fast range (>100 keV)

Case 2
- “URR Case”
- Moderated, copper reflected
- Maximize ^{95}Mo(n,γ) sensitivity in URR (2 keV – 200 keV)

Case 3
- “URR Void Case”
- Same as Case 3 but with molybdenum voids

Case 4
- “Epithermal Case”
- Moderated, copper reflected
- Maximize ^{95}Mo(n,γ) sensitivity in epithermal range (0.625 eV – 2 keV)

Case 5
- “Thermal Case”
- Moderated, copper reflected
- Maximize ^{95}Mo(n,γ) sensitivity in thermal range (<0.625 eV)

Energy

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Case 1 – Fast Case (>100 keV)

- Goal: Unmoderated, copper reflected, molybdenum HEU system with maximum molybdenum sensitivity in the fast energy region (100 keV – 20 MeV)

$$S_{k_{eff},\sigma_{fast}} = \int_{100\ keV}^{20\ MeV} \frac{\Delta k_{eff}/k_{eff}}{\Delta\sigma(E)/\sigma(E)}\, dE$$

- Covers upper range of RPI molybdenum measurements (1 keV – 620 keV)

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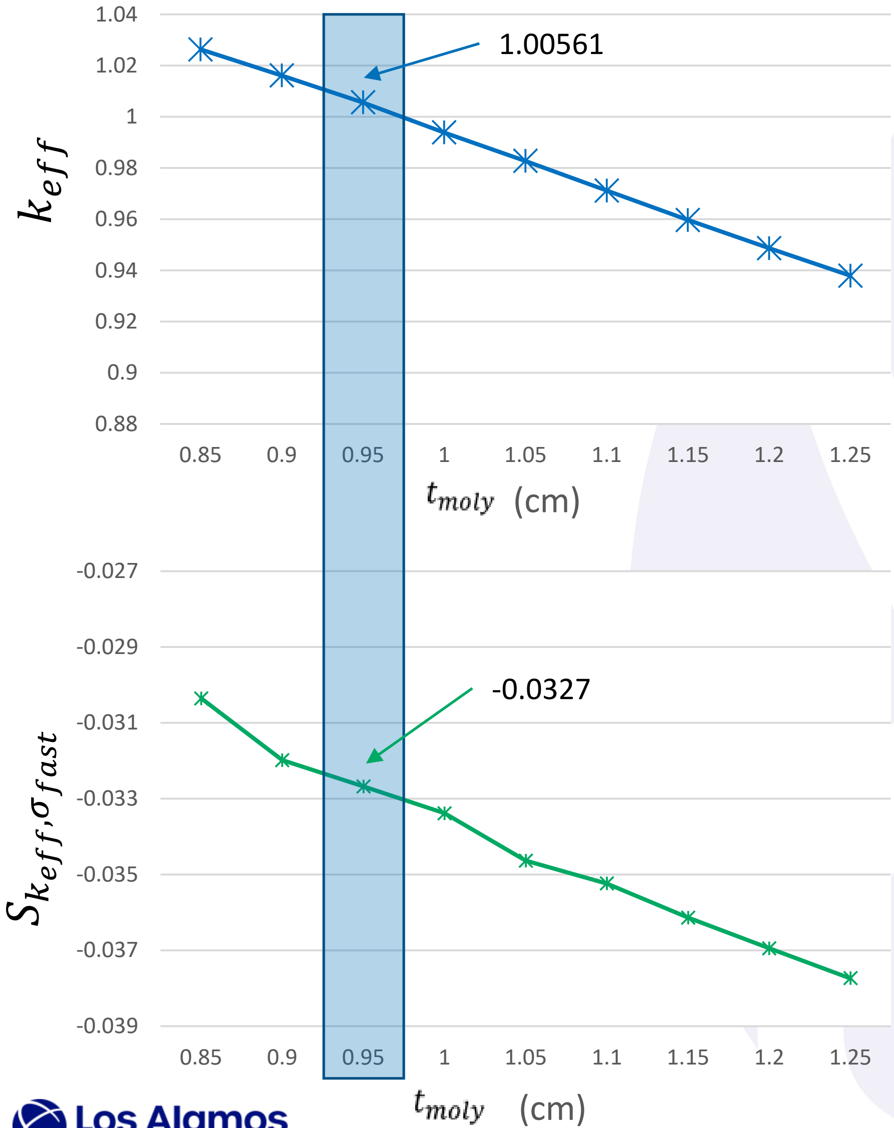
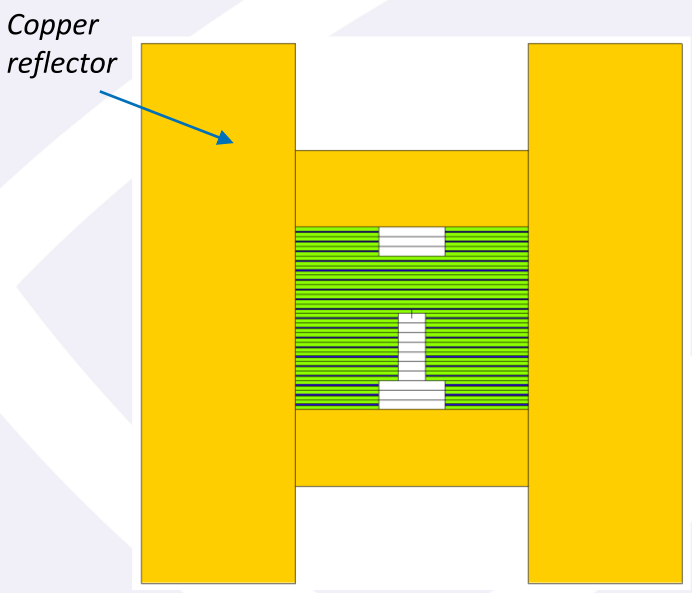
Case 1 – Fast Case (>100 keV)

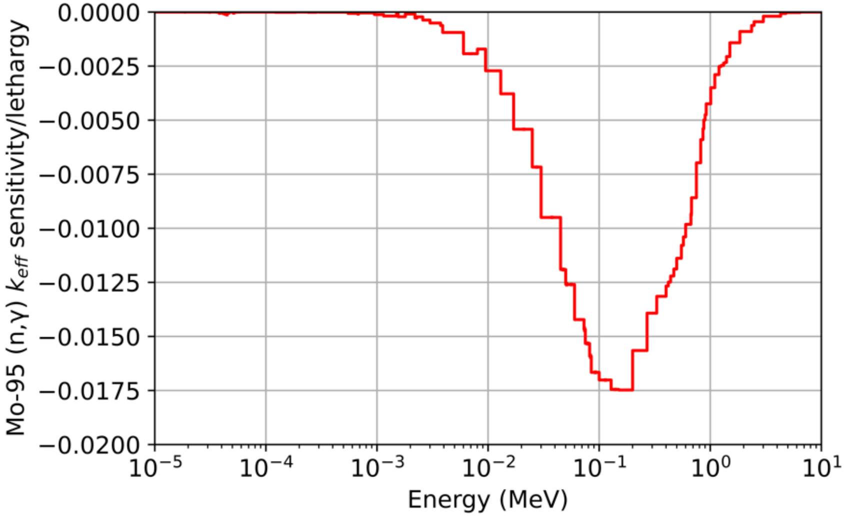


Case 1 Unit Geometry

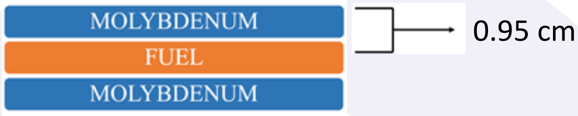


Case 1 Geometry (20 units)

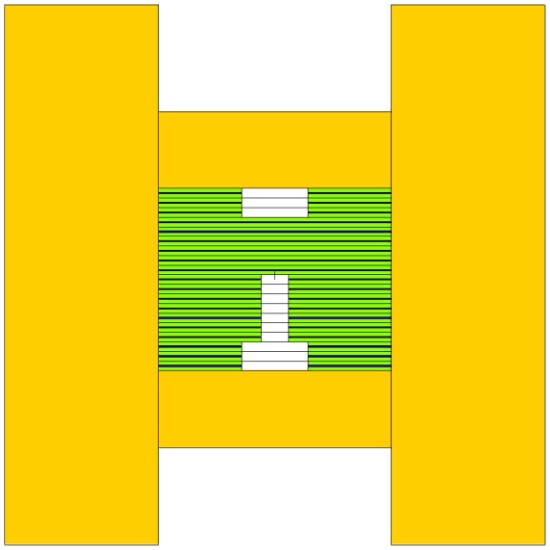
Proposed Case 1 – Fast Case (>100 keV)



Case 1 ^{95}Mo(n,γ) sensitivity



Case 1 Unit Geometry



Case 1 Geometry (20 units)

Case 2 – URR Case (2 keV – 200 keV)

- Goal: Maximize $^{95}Mo(n,\gamma)$ sensitivity in URR (2 keV – 200 keV)

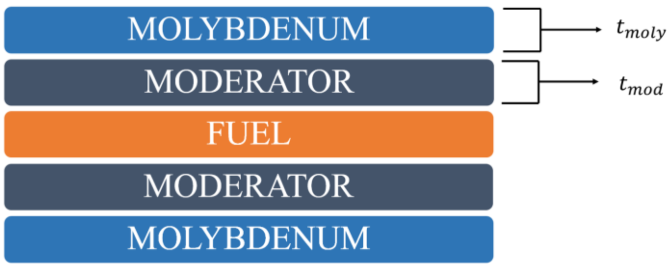
$$S_{k_{eff},\sigma_{URR}} = \int_{2\ keV}^{200\ keV} \frac{\Delta k_{eff} / k_{eff}}{\Delta\sigma(E) / \sigma(E)} dE$$

- The moderator that provides the highest sensitivity for this case will be used in the “URR Void Case” as well

- Covers lower range of RPI molybdenum measurements (1 keV – 620 keV)

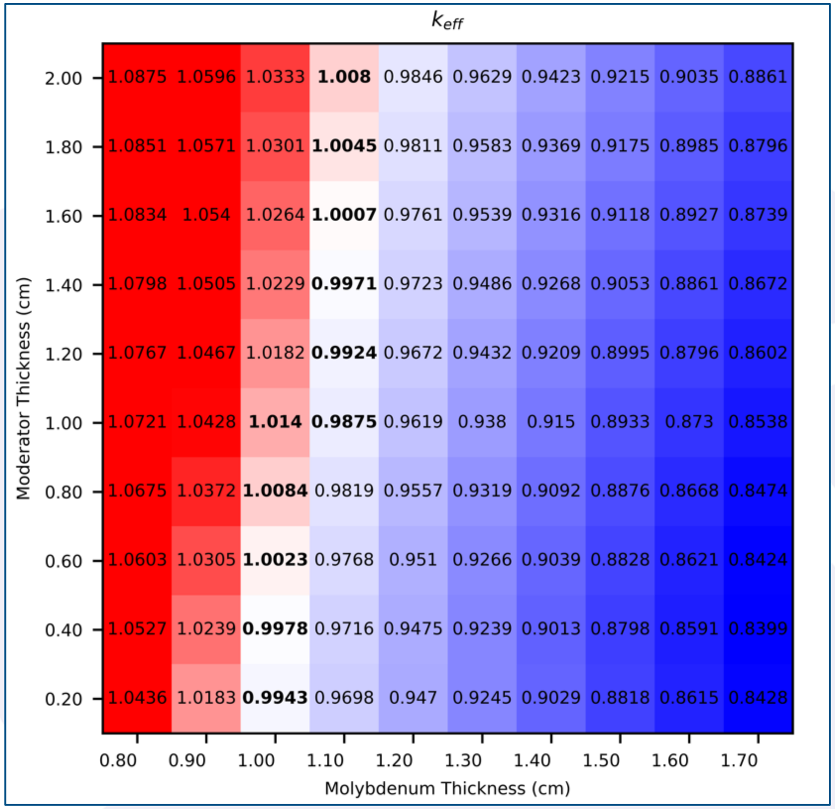
- Almost complete lack of benchmarks sensitive at this energy

Optimization Method



- The thickness of the molybdenum and moderator plates (t_{moly}, t_{mod}) are varied over a range of values to optimize a system parameter (i.e. $S_{k,x}$ or k_{eff})

- Four moderators are being investigated



Arbitrary moderator vs. molybdenum thickness plot

Alumina	Beryllium	Polyethylene	Teflon
Al_2O_3	Be	C_2H_4	C_2F_4

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k_{eff} of various configurations (2 keV – 200 keV)

Alumina

Alumina Thickness (cm) \ Molybdenum Thickness (cm)	0.60	0.65	0.70	0.75	0.80	0.85	0.90	0.95	1.00	1.05
1.20	**0.9972**	0.9824	0.9683	0.9549	0.9417	0.9287	0.9162	0.9039	0.8925	0.8813
1.10	**1.0046**	**0.9901**	0.9758	0.9626	0.9496	0.9368	0.9244	0.912	0.8995	0.8884
1.00	1.0128	**0.9992**	0.9844	0.9712	0.9568	0.9444	0.932	0.9198	0.9081	0.8961
0.90	1.022	**1.0073**	**0.9929**	0.9796	0.9657	0.9532	0.9398	0.9273	0.9157	0.9036
0.80	1.0295	1.0155	**1.0015**	0.9879	0.9745	0.9612	0.9489	0.9356	0.9237	0.912
0.70	1.0389	1.025	1.0108	**0.9972**	0.9835	0.9702	0.9578	0.9452	0.9324	0.92
0.60	1.0481	1.0331	1.0201	**1.0055**	**0.9925**	0.9794	0.9665	0.9541	0.9407	0.9292
0.50	1.0553	1.0421	1.0288	1.0153	**1.0018**	0.9895	0.976	0.9633	0.9512	0.939
0.40	1.0635	1.0507	1.0372	1.0239	1.0115	**0.9979**	0.9853	0.9728	0.9601	0.9478
0.30	1.0705	1.0581	1.0455	1.0322	1.0194	**1.0067**	**0.9948**	0.9815	0.9696	0.9572

Beryllium

Beryllium Thickness (cm) \ Molybdenum Thickness (cm)	0.85	0.90	0.95	1.00	1.05	1.10	1.15	1.20	1.25	1.30
1.30	1.0511	1.0358	1.0224	**1.0089**	**0.9951**	0.9818	0.9689	0.9568	0.9442	0.9321
1.20	1.0499	1.035	1.0207	**1.0065**	**0.9932**	0.9807	0.9673	0.9547	0.9426	0.9305
1.10	1.0475	1.0333	1.0184	**1.005**	**0.9909**	0.978	0.9656	0.9532	0.9401	0.9285
1.00	1.0467	1.0316	1.0168	**1.0024**	0.9895	0.9759	0.9632	0.9496	0.9379	0.9257
0.90	1.0443	1.029	1.0153	**1.0003**	0.9862	0.9735	0.9602	0.9482	0.9359	0.9235
0.80	1.0421	1.027	1.0122	**0.9979**	0.9842	0.9709	0.9581	0.9452	0.9329	0.9207
0.70	1.0401	1.0248	1.0101	**0.9959**	0.982	0.9686	0.9549	0.9424	0.9308	0.9185
0.60	1.0369	1.0224	**1.0077**	**0.994**	0.9802	0.9665	0.9533	0.9411	0.9281	0.9157
0.50	1.0348	1.0205	**1.0055**	**0.9921**	0.9776	0.9642	0.951	0.9387	0.9263	0.9143
0.40	1.0348	1.0189	**1.0045**	0.9899	0.9762	0.963	0.9502	0.9374	0.9256	0.9137

Polyethylene

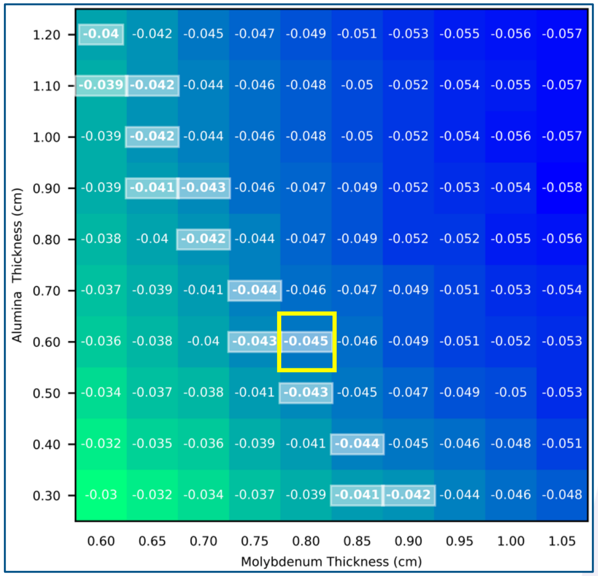
Polyethylene Thickness (cm) \ Molybdenum Thickness (cm)	1.00	1.20	1.40	1.60	1.80	2.00	2.20	2.40	2.60	2.80
1.00	1.2348	1.1939	1.156	1.1216	1.0888	1.0594	1.0324	**1.0064**	0.9834	0.962
0.90	1.234	1.1917	1.1535	1.1179	1.0845	1.0543	1.0256	**0.9986**	0.9752	0.9525
0.80	1.2285	1.1855	1.1467	1.1109	1.0772	1.0453	1.0158	0.9891	0.9636	0.9406
0.70	1.2193	1.1756	1.136	1.099	1.0651	1.0329	**1.002**	0.9744	0.9485	0.9239
0.60	1.2055	1.1612	1.1204	1.0834	1.0485	1.0153	0.985	0.9553	0.9283	0.904
0.50	1.1855	1.1409	1.0998	1.0621	1.0262	**0.9922**	0.9618	0.932	0.9032	0.8775
0.40	1.1588	1.1134	1.0717	1.0332	**0.9967**	0.9635	0.9315	0.9008	0.8726	0.8454
0.30	1.1241	1.0784	1.0364	**0.997**	0.9592	0.9251	0.8933	0.8622	0.8326	0.8066
0.20	1.0813	1.0347	**0.9915**	0.9514	0.914	0.8789	0.8465	0.8153	0.7861	0.7585
0.10	1.0311	0.9839	0.9394	0.8983	0.8602	0.8254	0.7925	0.7612	0.7323	0.7052

Teflon

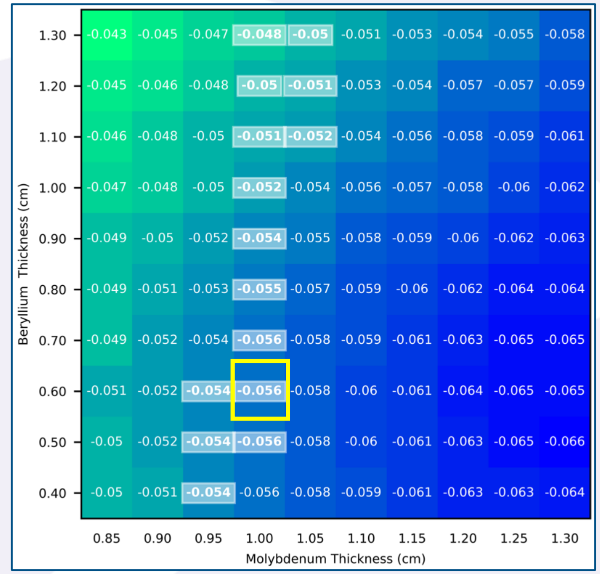
Teflon Thickness (cm) \ Molybdenum Thickness (cm)	0.10	0.20	0.30	0.40	0.50	0.60	0.70	0.80	0.90	1.00
2.50	0.9774	0.9461	0.9167	0.8897	0.8639	0.8408	0.8183	0.7968	0.7776	0.7608
2.25	**1.0002**	0.9697	0.9406	0.9123	0.8868	0.8617	0.8383	0.8166	0.7958	0.7767
2.00	1.0222	**0.9916**	0.9635	0.9364	0.9098	0.8849	0.8608	0.8382	0.8165	0.7955
1.75	1.0426	1.0126	0.9842	0.958	0.9326	0.9075	0.884	0.8605	0.838	0.8166
1.50	1.063	1.0345	**1.0061**	0.9803	0.9545	0.9295	0.9058	0.883	0.861	0.8383
1.25	1.0844	1.0565	1.0303	**1.0032**	0.9773	0.9526	0.9284	0.906	0.8834	0.8615
1.00	1.1036	1.0796	1.0542	1.0282	**1.0028**	0.9775	0.9533	0.9296	0.9069	0.8844
0.75	1.119	1.1004	1.0777	1.0538	1.0292	**1.0048**	0.9803	0.9554	0.9322	0.9094
0.50	1.1257	1.1144	1.0984	1.0779	1.0554	1.032	**1.0079**	0.9839	0.96	0.937
0.25	1.1257	1.1158	1.1088	1.0961	1.0781	1.0583	1.0357	1.0124	0.9896	0.9658

$S_{k_{eff},\sigma_{URR}}$ of various configurations (2 keV – 200 keV)

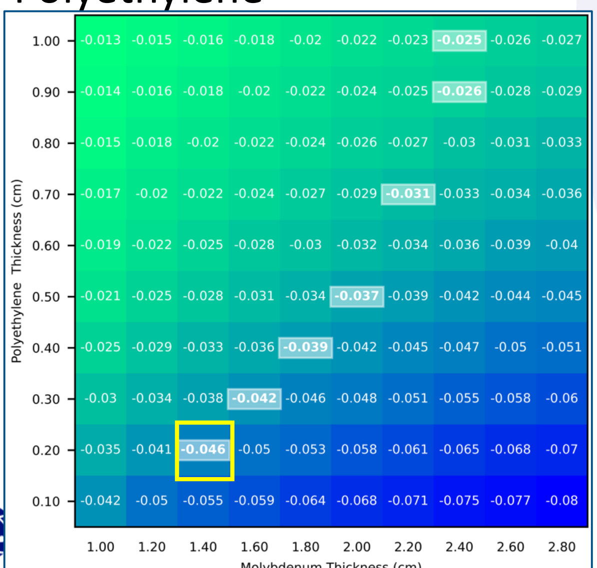
Alumina



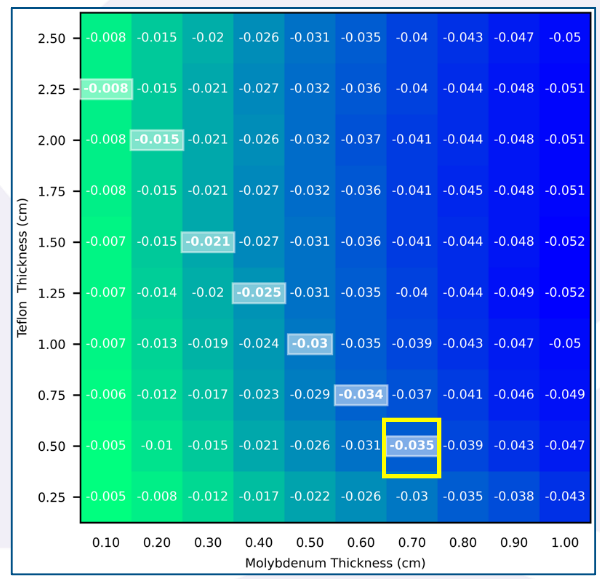
Beryllium



Polyethylene

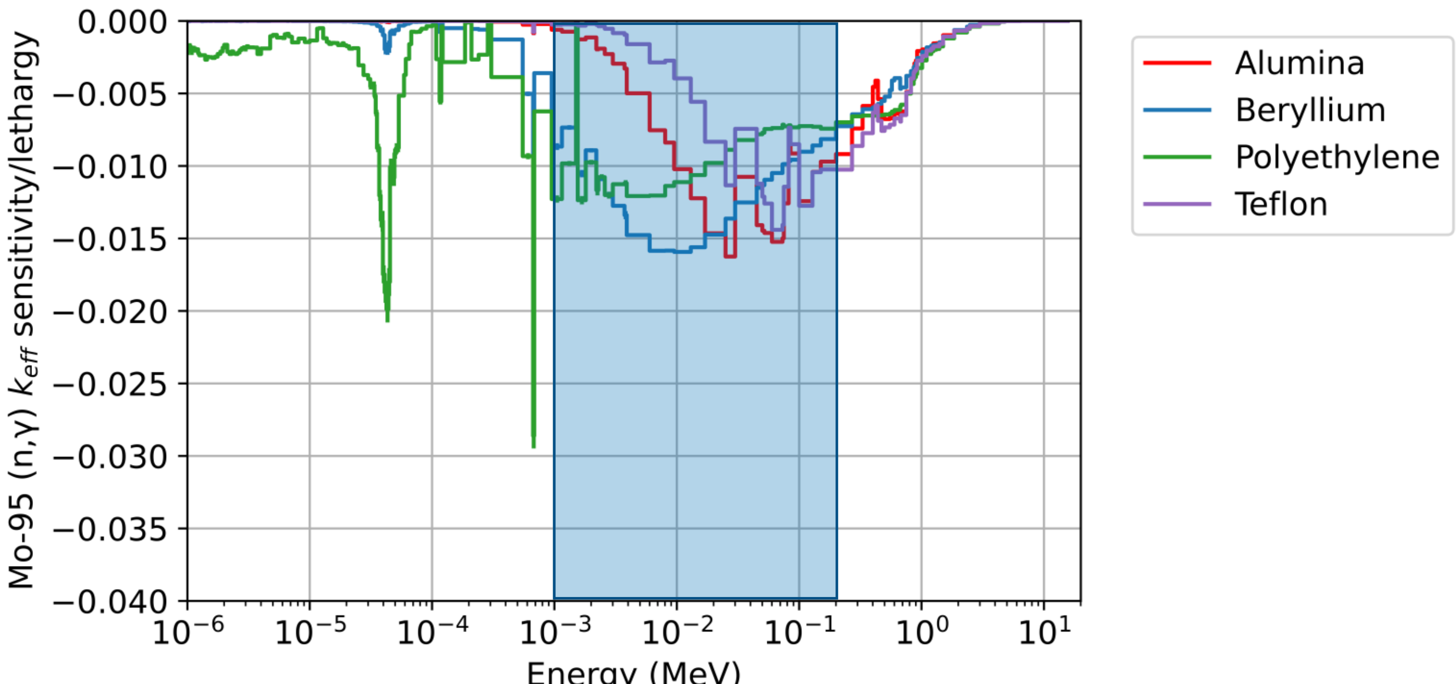


Teflon

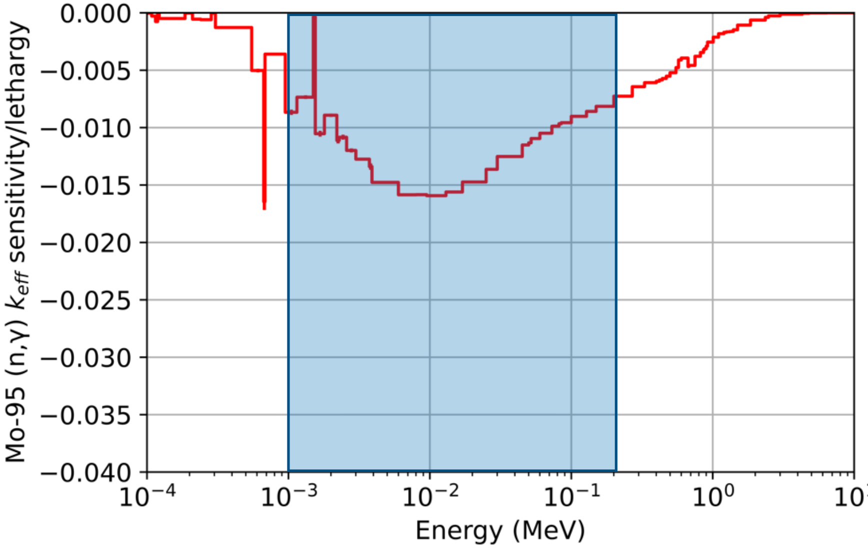


Investigated URR Moderators (2 keV – 200 keV)

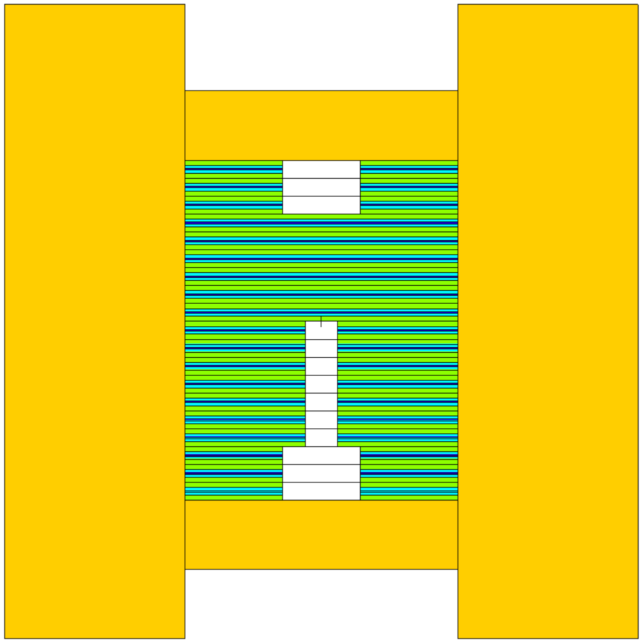
Moderator	Alumina	Beryllium	Polyethylene	Teflon
Formula	Al_2O_3	Be	C_2H_4	C_2F_4
Density [$\frac{g}{cm^3}$]	3.97	1.848	0.93	2.25
$S_{k_{eff},\sigma_{URR}}$	-0.045	-0.056	-0.046	-0.035
$t_{moly}[cm]$	0.8	1.0	1.4	0.7
$t_{mod}[cm]$	0.6	0.6	0.2	0.5



Proposed Case 2 – URR Case (2 keV – 200 keV)



Moderator	Beryllium
Formula	Be
Density $[\frac{g}{cm^3}]$	1.848
$S_{k_{eff},\sigma_{Thermal}}$	-0.056
$t_{moly}[cm]$	1.0
$t_{mod}[cm]$	0.6



Case 3 – URR Void Case

- Goal: Create near identical system as Case 2 but with varying voids in central molybdenum plates
- Similar methodology to the lead voids in the Zeus experiments at NCERC
- Data can be used by evaluators to establish trends in C/E values as molybdenum mass is removed

Case 4 – Epithermal Case (0.625 eV – 2 keV)

- Goal: Moderated, copper reflected, molybdenum HEU system with maximum molybdenum sensitivity in the epithermal energy region (0.625 eV - 2 keV)

$$S_{k_{eff},\sigma_{fast}} = \int_{0.625\ eV}^{2\ keV} \frac{\Delta k_{eff} / k_{eff}}{\Delta\sigma(E) / \sigma(E)} dE$$

Alumina	Beryllium	Polyethylene	Teflon

- Covers upper range of J-PARC molybdenum measurements (0 eV – 600 eV)

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k_{eff} of various configurations (0.625 eV – 2 keV)

Alumina

Alumina Thickness (cm) \ Molybdenum Thickness (cm)	0.10	0.20	0.30	0.40	0.50	0.60	0.70	0.80	0.90	1.00
3.10	1.0297	**0.9911**	0.9569	0.9267	0.8988	0.8726	0.8487	0.8263	0.8056	0.7857
2.80	1.0515	1.0116	0.9771	0.9459	0.9162	0.8898	0.8649	0.8417	0.8201	0.7995
2.50	1.0732	1.0323	**0.9972**	0.9649	0.9353	0.908	0.8817	0.8576	0.8349	0.8139
2.20	1.0945	1.0535	1.0178	0.9852	0.9546	0.9267	0.9002	0.8756	0.8522	0.8305
1.90	1.1163	1.0752	1.0395	**1.0058**	0.9746	0.9459	0.9193	0.8936	0.87	0.8474
1.60	1.1386	1.0977	1.0611	1.0275	**0.9957**	0.9663	0.9393	0.9136	0.8889	0.8654
1.30	1.159	1.1195	1.0839	1.0501	1.0186	0.9883	0.9605	0.9347	0.9093	0.8858
1.00	1.178	1.1414	1.1077	1.0748	1.0426	1.0128	0.9844	0.9568	0.932	0.9081
0.70	1.1886	1.1586	1.1283	1.0985	1.0679	1.0389	1.0108	0.9835	0.9578	0.9324
0.40	1.1765	1.1604	1.1401	1.1155	1.0903	1.0635	1.0372	1.0115	0.9853	0.9601

Beryllium

Beryllium Thickness (cm) \ Molybdenum Thickness (cm)	0.80	0.85	0.90	0.95	1.00	1.05	1.10	1.15	1.20	1.25
1.75	1.0707	1.056	1.041	1.0285	1.0154	**1.0028**	0.9896	0.9777	0.9658	0.9546
1.65	1.0695	1.0544	1.0404	1.027	1.014	**1.0007**	0.9888	0.9771	0.9647	0.9533
1.55	1.0692	1.054	1.0404	1.0257	1.0126	**0.9992**	0.9868	0.9742	0.9625	0.9509
1.45	1.0674	1.0527	1.0388	1.025	1.0107	**0.9979**	0.9851	0.9724	0.9602	0.9486
1.35	1.0667	1.0519	1.037	1.0231	**1.0095**	**0.9962**	0.9827	0.9706	0.9586	0.9466
1.25	1.0657	1.051	1.0363	1.0215	**1.0078**	**0.9943**	0.9811	0.9692	0.9564	0.9444
1.15	1.0642	1.0485	1.034	1.0197	**1.0049**	**0.9922**	0.9792	0.9661	0.9531	0.9415
1.05	1.0624	1.0474	1.0327	1.0176	**1.0041**	**0.9902**	0.9771	0.9641	0.9517	0.9397
0.95	1.0607	1.0449	1.0304	1.0156	**1.0012**	0.9881	0.975	0.9622	0.9491	0.9369
0.85	1.0587	1.0436	1.0287	1.0136	**0.9989**	0.9858	0.9723	0.9598	0.9464	0.9343

Polyethylene

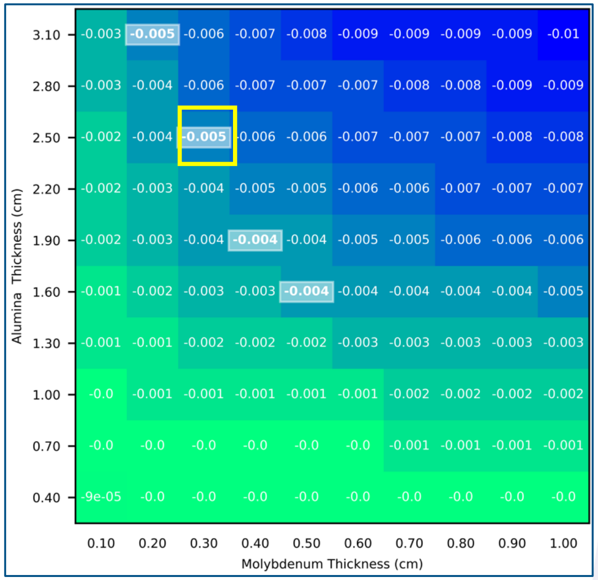
Polyethylene Thickness (cm) \ Molybdenum Thickness (cm)	1.00	1.20	1.40	1.60	1.80	2.00	2.20	2.40	2.60	2.80
1.00	1.2348	1.1939	1.156	1.1216	1.0888	1.0594	1.0324	**1.0064**	0.9834	0.962
0.90	1.234	1.1917	1.1535	1.1179	1.0845	1.0543	1.0256	**0.9986**	0.9752	0.9525
0.80	1.2285	1.1855	1.1467	1.1109	1.0772	1.0453	1.0158	0.9891	0.9638	0.9406
0.70	1.2193	1.1756	1.138	1.099	1.0651	1.0329	**1.002**	0.9744	0.9485	0.9239
0.60	1.2055	1.1612	1.1204	1.0834	1.0485	1.0153	0.985	0.9553	0.9283	0.904
0.50	1.1855	1.1409	1.0998	1.0621	1.0262	**0.9922**	0.9618	0.932	0.9032	0.8775
0.40	1.1588	1.1134	1.0717	1.0332	**0.9967**	0.9635	0.9315	0.9008	0.8726	0.8454
0.30	1.1241	1.0784	1.0364	**0.997**	0.9592	0.9251	0.8933	0.8622	0.8326	0.8066
0.20	1.0813	1.0347	**0.9915**	0.9514	0.914	0.8789	0.8465	0.8153	0.7861	0.7585
0.10	1.0311	0.9839	0.9394	0.8983	0.8602	0.8254	0.7925	0.7612	0.7323	0.7052

Teflon

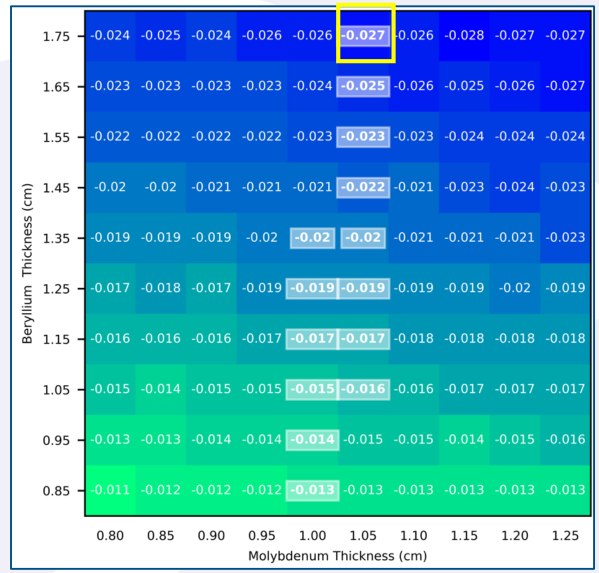
Teflon Thickness (cm) \ Molybdenum Thickness (cm)	0.10	0.20	0.30	0.40	0.50	0.60	0.70	0.80	0.90	1.00
2.50	0.9774	0.9461	0.9167	0.8897	0.8639	0.8408	0.8183	0.7968	0.7776	0.7608
2.25	**1.0002**	0.9697	0.9406	0.9123	0.8868	0.8617	0.8383	0.8166	0.7958	0.7767
2.00	1.0222	**0.9916**	0.9635	0.9364	0.9098	0.8849	0.8608	0.8382	0.8165	0.7955
1.75	1.0426	1.0126	0.9842	0.958	0.9326	0.9075	0.884	0.8605	0.838	0.8166
1.50	1.063	1.0345	**1.0061**	0.9803	0.9545	0.9295	0.9058	0.883	0.861	0.8383
1.25	1.0844	1.0565	1.0303	**1.0032**	0.9773	0.9526	0.9284	0.9056	0.8834	0.8615
1.00	1.1036	1.0796	1.0542	1.0282	**1.0028**	0.9775	0.9533	0.9296	0.9069	0.8844
0.75	1.119	1.1004	1.0777	1.0538	1.0292	**1.0048**	0.9803	0.9554	0.9328	0.9094
0.50	1.1257	1.1144	1.0984	1.0779	1.0554	1.032	**1.0079**	0.9839	0.96	0.937
0.25	1.1257	1.1158	1.1088	1.0961	1.0781	1.0583	1.0357	1.0124	0.9896	0.9658

$S_{k_{eff},\sigma_{Epithermal}}$ of various configurations (0.625 eV – 2 keV)

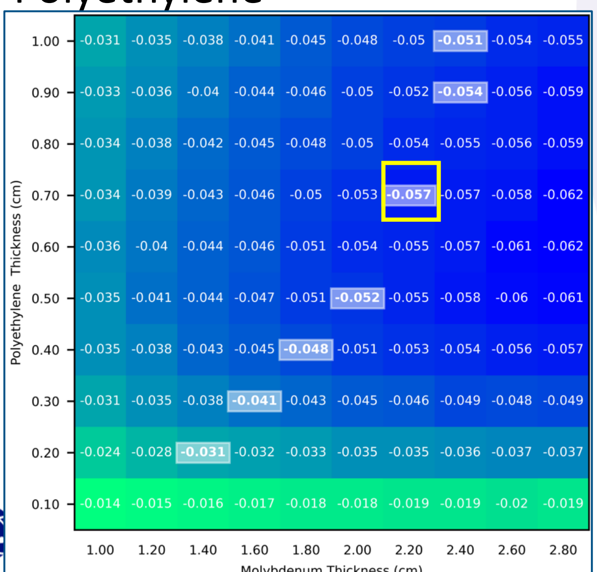
Alumina



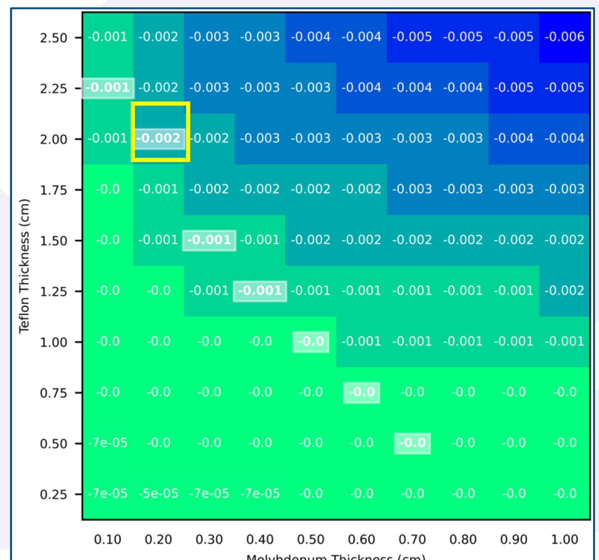
Beryllium



Polyethylene

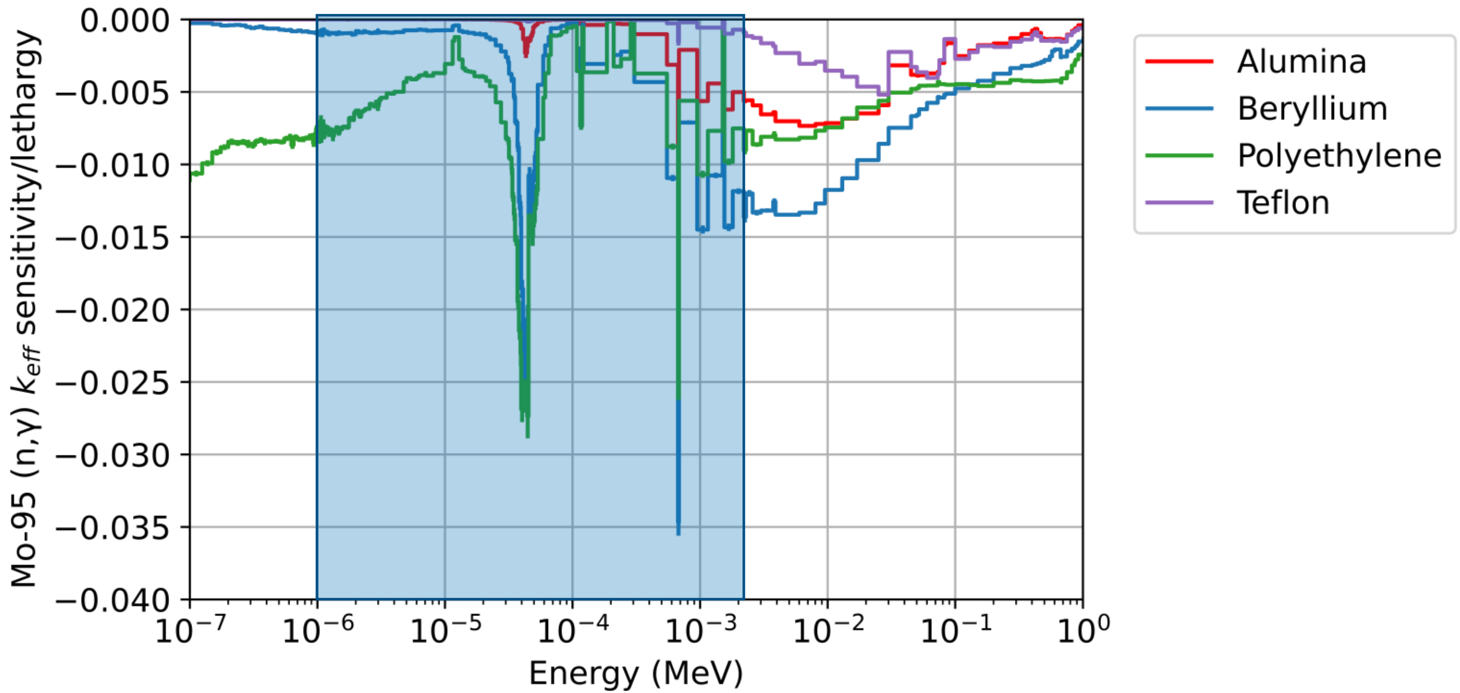


Teflon

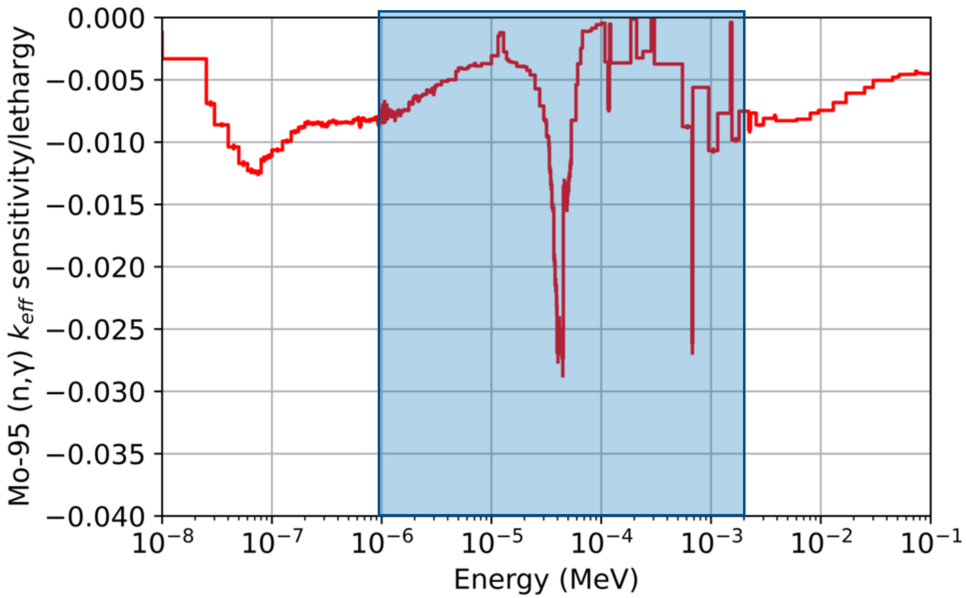


Investigated Epithermal Moderators (0.625 eV – 2 keV)

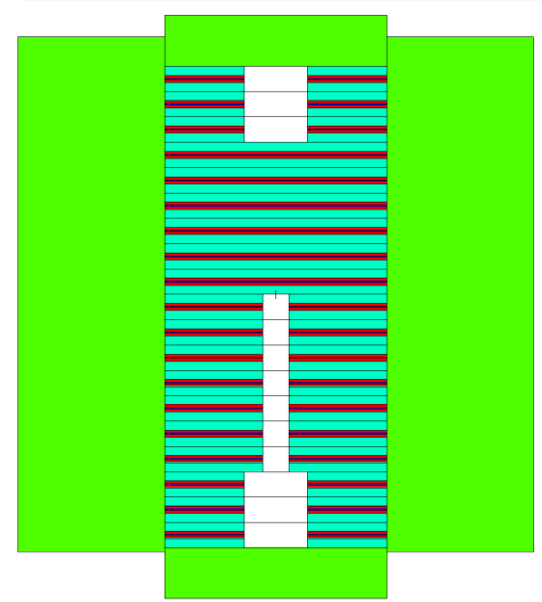
Moderator	Alumina	Beryllium	Polyethylene	Teflon
Formula	Al_2O_3	Be	C_2H_4	C_2F_4
Density $[\frac{g}{cm^3}]$	3.97	1.848	0.93	2.25
$S_{k_{eff},\sigma_{Epithermal}}$	-0.005	-0.027	-0.057	-0.002
$t_{moly}[cm]$	0.3	1.05	2.2	0.2
$t_{mod}[cm]$	2.5	1.75	0.7	2.0



Proposed Case 4 – Epithermal Case (0.625 eV – 2 keV)



Moderator	Polyethylene
Formula	C_2H_4
Density $[\frac{g}{cm^3}]$	0.93
$S_{k_{eff},\sigma_{Epithermal}}$	-0.057
$t_{moly}[cm]$	2.2
$t_{mod}[cm]$	0.7



Case 5 – Thermal Case (<0.625 eV)

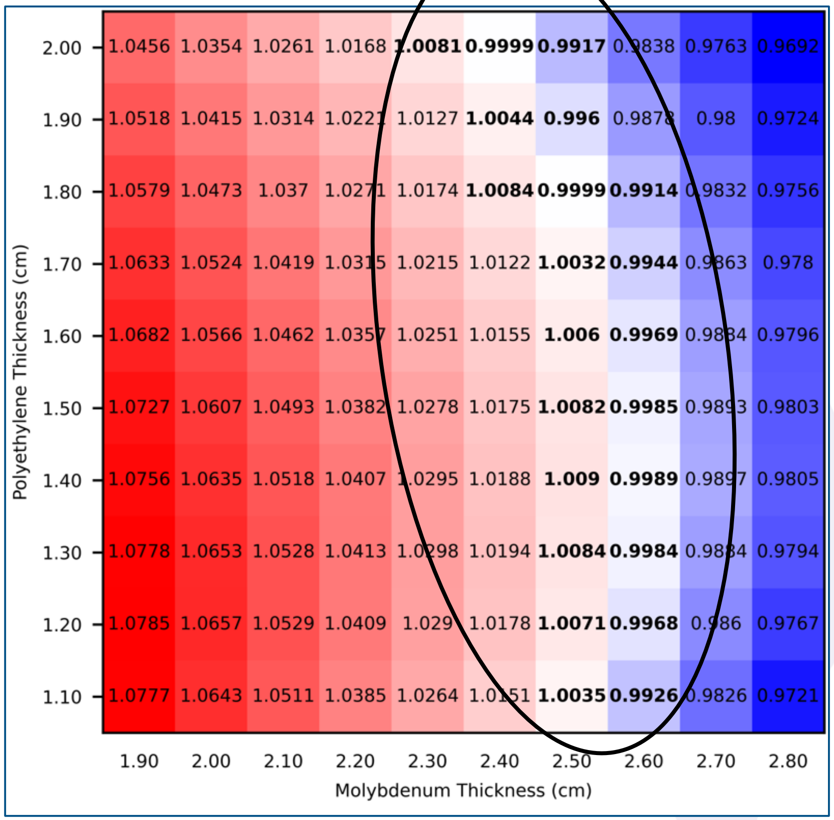
- Goal: Moderated, copper reflected, molybdenum HEU system with maximum molybdenum sensitivity in the thermal energy region (<0.625 eV)

$$S_{k_{eff},\sigma_{fast}} = \int_{0.0\ eV}^{0.625\ keV} \frac{\Delta k_{eff}/k_{eff}}{\Delta\sigma(E)/\sigma(E)} dE$$

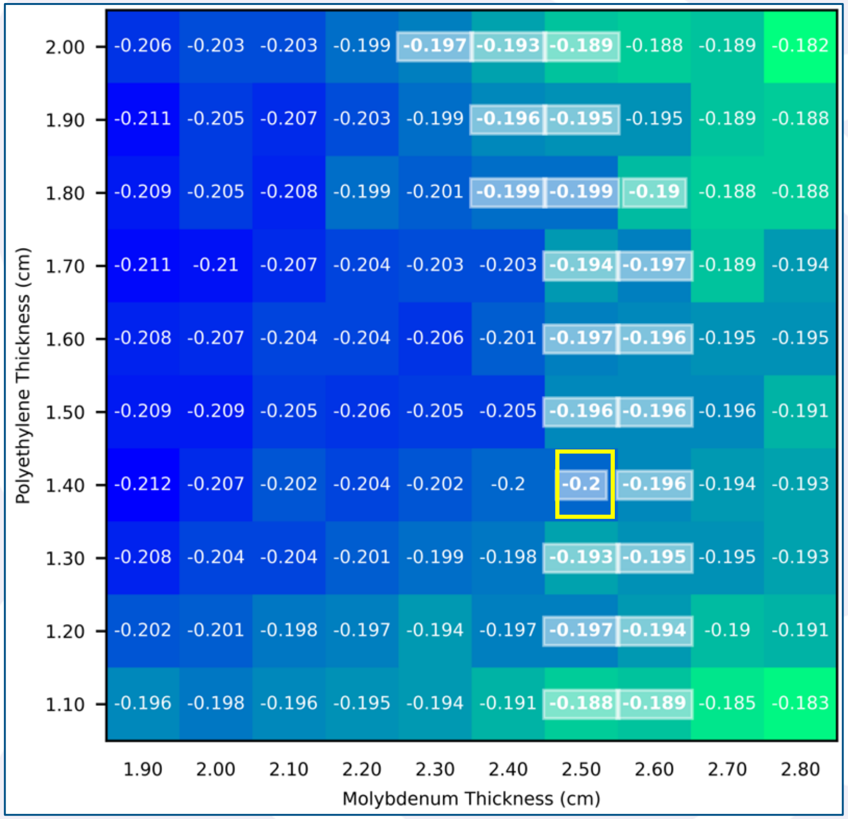
- Covers lower range of J-PARC molybdenum measurements (0 eV – 600 eV)

Thermal polyethylene configurations (<0.625 eV)

k_{eff}



$S_{k_{eff},\sigma_{Thermal}}$



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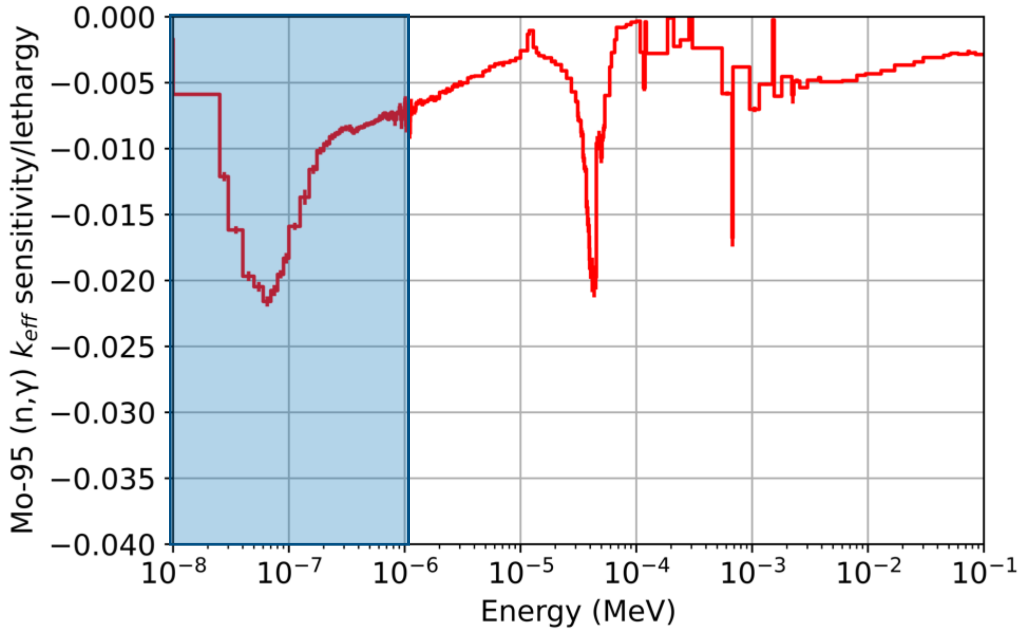
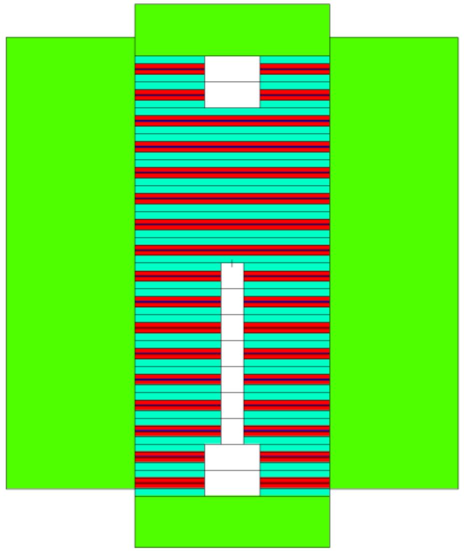
Proposed Case 5 – Thermal Case (<0.625 eV)

Moderator	Polyethylene
Formula	C_2H_4
Density $[\frac{g}{cm^3}]$	0.93
$S_{k_{eff},\sigma_{Thermal}}$	-0.057
$t_{moly}[cm]$	2.5
$t_{mod}[cm]$	1.4





Review

Fast (x1)

MOLYBDENUM
FUEL
MOLYBDENUM

- **Case 1**
- Unmoderated, copper reflected
- "Fast Case"

Intermediate (x3)

MOLYBDENUM
MODERATOR
FUEL
MODERATOR
MOLYBDENUM

- **Case 2**
- Moderated, copper reflected
- Maximize ^{95}Mo(n,γ) sensitivity in URR (2 keV – 200 keV)
- "URR Case"

- **Case 3**
- Moderated, copper reflected
- Same as Case 3 but with molybdenum voids
- "URR Void Case"

- **Case 4**
- Moderated, copper reflected
- Maximize ^{95}Mo(n,γ) sensitivity in epithermal range (0.625 eV – 2 keV)
- "Epithermal Case"

Thermal (x1)

MOLYBDENUM
MODERATOR
FUEL
MODERATOR
MOLYBDENUM

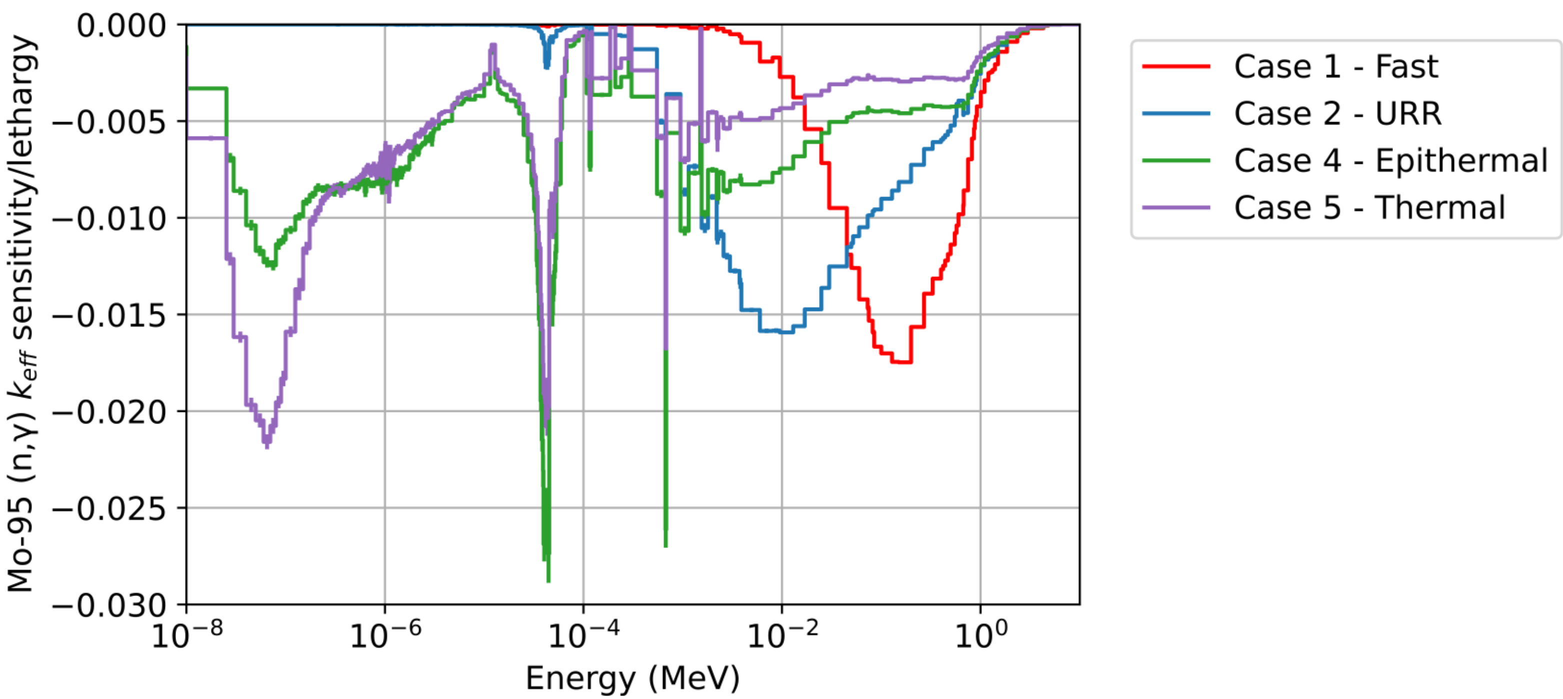
- **Case 5**
- Moderated, copper reflected
- Maximize ^{95}Mo(n,γ) sensitivity in thermal range (<0.625 eV)
- "Thermal Case"

Beryllium moderated (?)

Polyethylene moderated

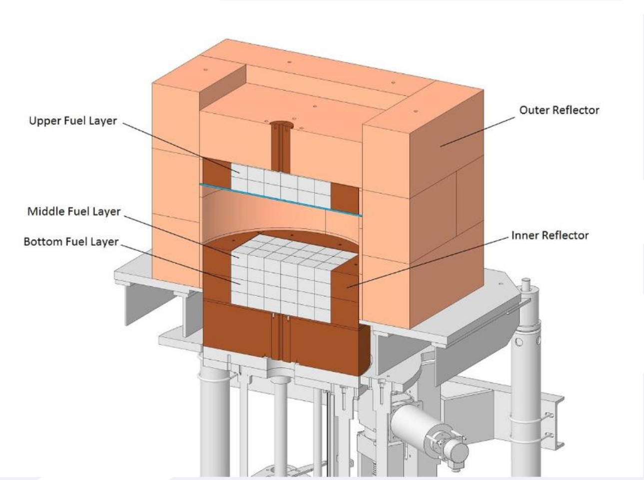
Review

	Case 1 "Fast"	Case 2 "URR"	Case 3 "Void URR"	Case 4 "Epithermal'	Case 5 "Thermal"
Moderator	N/A	Beryllium	Beryllium	Polyethylene	Polyethylene
$t_{moly}[cm]$	0.95	1.0	TBD	2.2	2.5
$t_{mod}[cm]$	N/A	0.6	TBD	0.7	1.4
Optimized Energy Range	>100 keV	2 keV – 200 keV	2 keV – 200 keV	0.626 eV – 2 keV	< 0.625 eV
Differential Data	RPI	RPI	RPI	J-PARC	J-PARC

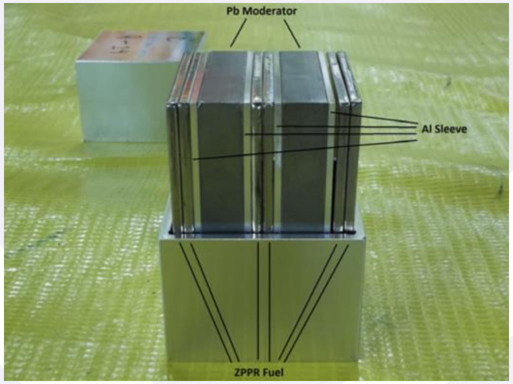


Future Work - Plutonium Cases

- Similar geometry to the Zeus plutonium/lead experiments
- ^{239}Pu ZPPR plates, molybdenum, and moderator fuel units reflected by copper
- Introduce voids by removing molybdenum in fuel units



Zeus Pu/Pb experiment on COMET



Fuel unit

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Future Work - Other Considerations

- Activation foils
- Neutron noise measurements (Rossi-α)
- Subcritical experiments

Proposed Experiment Name

- **<u>M</u>**olybdenum **<u>O</u>**ptimized **<u>B</u>**enchmark S**<u>y</u>**stem **<u>D</u>**emonstrating **<u>I</u>**ntegral **<u>C</u>**orrelations

- **MOBY DICK**

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Questions?

Extra Slides

^{95}Mo(n,γ) cross section